Surface Kondo Effect and Non-Trivial Metallic State of the Kondo Insulator YbB₁₂

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1. Introduction

Recently, non-trivial topology of the electronic states on Kondo insulator (KI), namely topological Kondo insulator (TKI) [1], is one of hot topics in physics. SmB₆, a well-known KI, is firstly investigated as a candidate of TKI. Earlier angle-resolved photoelectron spectroscopy (ARPES) experiments revealed metallic surface states on SmB₆ [2], but its origin and the topological order of SmB₆ is still under debate [3]. Therefore, a survey of another material is desirable to provide further insight into the topological origin of metallic surface states on KIs.

Ytterbium dodecaboride (YbB₁₂) is another typical KI which has a NaCl-type crystal structure with Yb and B₁₂ clusters [4]. A clear energy gap appears in the bulk of YbB₁₂ with a gap size of about 40 meV of the peak (15 meV of the onset) observed by an optical conductivity measurement [5]. However, finite density of states (DOS) at the Fermi level has been observed at ultra-low temperature by angle "integrated" photoelectron spectroscopy and this is considered to originate from a metallic surface state, and this metallic surface state also has been confirmed by using electrical transport measurements [6]. So, surface state of YbB₁₂ is attractive target for detailed research of topological surface state on TKI. But, the band dispersion of YbB₁₂ has not been observed by momentum-resolved measurements such as angle-resolved photoelectron spectroscopy (ARPES) because a well-defined clean surface has not been obtained [7].

In this work, we establish the method to obtain welldefined clean surface of another Kondo insulator YbB₁₂(001) and perform high-resolution ARPES experiments of the surface electronic structure.

2. Experimental

Whole photoemission experiments were performed at BL-2A MUSASHI of PF. We prepared a well-ordered surfaces of YbB₁₂ (001) by following procedure. Firstly, we mechanically polished the sample then heated it up to 1600 K with good pressure below 5.0×10^{-7} Pa in preparation chamber at the BL-2A end station. We confirmed the clean surface by wide valence band measurement. Figure 1 shows the result. These electronic structure especially at 2-4 eV, in which "surface"

components of Yb^{2+} disappear, corresponds to that of clean surface which our previous works reveal.

3. Results and Discussion

Figure 3 is band dispersions along [100] (direction is indicated in Fig. 2 bulk and surface Brillouin zone of YbB₁₂). A band with steep dispersion below 100 meV would be a conduction band. This band becomes less dispersive around 40 meV, probably due to the hybridization with localized Yb²⁺ 4*f* bands. Such hybridization between conduction and 4*f* bands would be driven by Kondo effect.

In addition to these states, we observed another state clearly crossing $E_{\rm F}$ at $k_{/[100]} \sim 0.18$ Å⁻¹ as indicated by MDC. This metallic surface state can be a cause of the remnant conduction path of YbB₁₂ observed by the transport experiment at low temperature [6]. This metallic state is also confirmed by MDC peaks attached to ARPES intensity plots of Fig. 3. In addition to this, we found another state dispersing in the gap formed by the bulk *c-f* hybridization, which connects the conduction band with

the metallic state at $\overline{\Gamma}$ and \overline{M} , which are time-reversal invariant momentum. These band characteristics such as continuous connection between valence and conduction band are satisfied with the necessary conditions of topological surface states.

Further study of this metallic state, especially its topological origin, is in progress.

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Fig. 1 Wide valence band spectrum of YbB₁₂.



Fig. 2 Bulk and surface Brillouin zones of YbB₁₂. The $c(2 \times 2)$ surface reconstruction has been confirmed by our previous experiments.



Fig. 3. ARPES intensity plots along [100] near E_F taken with 53.5 eV photons (bottom) and momentum distribution curves at E_F (±10 meV) (top). ARPES image was divided by Fermi-Dirac distribution function at the sample temperature of 20 K convolved with the instrumental resolution.